

Emergent Second Law in Pure Quantum States

Tatsuhiko N. Ikeda,¹ Naoyuki Sakumichi,¹ Anatoli Polkovnikov,² and Masahito Ueda¹

¹Department of Physics, University of Tokyo, Tokyo, 113-0033, Japan

²Physics Department, Boston University, Boston, MA 02215, USA

(Dated: March 25, 2013)

Phenomena around us seem to evolve only in the forward direction of time, despite the fact that the underlying microscopic laws of physics are invariant under time reversal apart from a certain rare interaction in particle physics [1]. This enigma concerning the arrow of time is naturally associated with the second law of thermodynamics, which dictates that the entropy of an isolated system never decrease [2]. The question of whether and, if so, how the second law emerges from quantum mechanics has long been tackled [3]. However, the current understanding remains unsatisfactory because most studies deal with open systems coupled to the surrounding environments where the time evolution of the system alone is no longer time-reversal symmetric [4–6]. Here we show that the second law emerges from an isolated pure quantum state through its unitary evolution. The physics behind the second law is the quantum-mechanical energy uncertainty associated with every finite-time operation that makes a large number of many-body energy eigenstates indistinguishable, resulting in a non-decreasing entropy of the system [7]. Our result establishes the quantum-mechanical definition of the thermodynamic entropy, opening up the way to study thermodynamics in isolated quantum systems, where persistent quantum coherence is expected to cause hitherto unexplored effects [8, 9]. In fact, independently of details of the system and processes, quantum coherence between many-body eigenstates is shown to bring about a universal many-body correction to the entropy. Such new effects are expected to be experimentally observed using ultra-cold atoms or ions [10–12].

The second law of thermodynamics asserts that the entropy of an isolated system never decreases during any thermodynamic process. On the other hand, quantum mechanics tells us that an isolated system is described by a pure quantum state and that its time evolution is unitary and hence reversible. Then, the crucial question is: can such a non-decreasing quantity emerge from pure quantum states?

We answer this question in the affirmative by proposing that the proper quantum-mechanical definition of the thermodynamic entropy is given by

$$S(\rho) = - \sum_n \rho_{nn} \ln \rho_{nn}, \quad (1)$$

where ρ_{nn} 's are the diagonal elements of the density

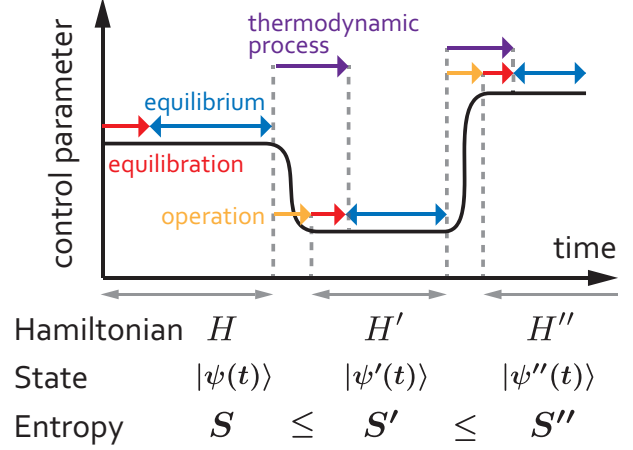


FIG. 1: **Summary of the main result.** With the control parameter in the Hamiltonian held fixed, the pure quantum state reaches equilibrium (blue). Then a thermodynamic process (purple), which consists of the operation (yellow) and equilibration (red), causes a transition to a different pure state at equilibrium. During the thermodynamic process, the entropy never decreases, $S \leq S'$. Since both the initial and final states are pure, repeated application of this argument leads to the second law of thermodynamics, $S \leq S' \leq S'' \leq \dots$.

matrix ρ in the eigenbasis of the Hamiltonian and Boltzmann's constant is set to unity [13, 14]. It quantifies the energy uncertainty and correctly describes the thermodynamic entropy. It is because it reduces to the von Neumann entropy for the canonical ensemble [13]. We note that the von Neumann entropy is inconsistent with the second law of thermodynamics because it is invariant under any unitary evolution in an isolated quantum system and vanishes for pure quantum states.

Before stating our main result, we recall the zeroth law of thermodynamics for pure quantum states, which states that a pure state reaches equilibrium under unitary evolution [15]. This fact has only recently been verified theoretically [16, 17] and experimentally [18], and the closely related result concerning quantum ergodicity has been unearthed [19]. For equilibration to occur, the pure state must involve a large number of energy eigenstates, which are coherently superposed.

Our main result is that the entropy (1) never decreases during any thermodynamic process in large systems as follows. Let a thermodynamic process be composed of the operation and equilibration, causing a transition between two pure states at equilibrium as

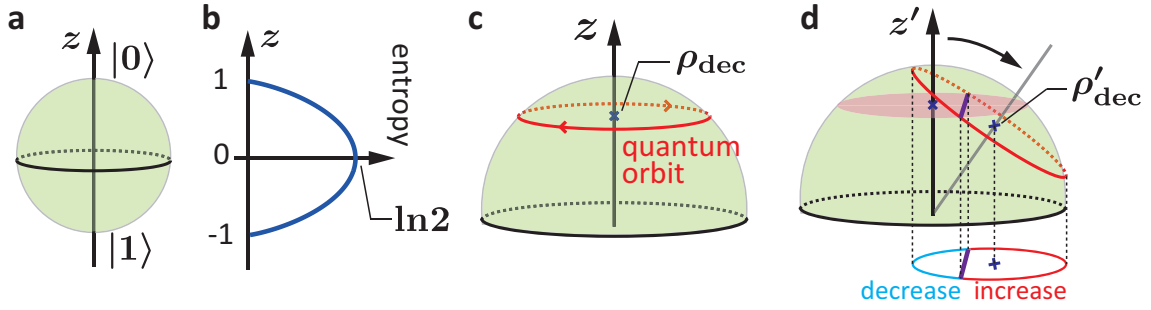


FIG. 2: **Geometrical interpretation of the entropy increase.** (a) Each density matrix is represented by a point on or inside the Bloch sphere. (b) The entropy (1) depends only on the z -component and attains the maximum value of $\ln 2$ on the equatorial plane. (c) A pure state traces a circular quantum orbit perpendicular to the z -axis under unitary evolution for a fixed Hamiltonian. The projection of this orbit onto the z -axis gives ρ_{dec} , which retains no coherence between $|0\rangle$ and $|1\rangle$. (d) A quantum operation and the associated change in the energy eigenbasis, which tilt the axis of the orbit. The entropy of the decohered state ρ'_{dec} increases during the process. The entropy increases for more than half of the pure states on the orbit.

illustrated in Fig. 1. A control parameter in the Hamiltonian, e.g. a magnetic field, is varied during the operation and kept constant during equilibration. Let S and S' denote the entropies before and after the thermodynamic process, respectively. Then, assuming a uniform distribution about the timing at which the operation is performed, we obtain

$$S \leq S' \quad (2)$$

for large systems with almost unit probability. The equality holds for quasistatic, or infinitely-slow, processes. Note that the initial state need not be assumed to belong to any special statistical ensemble such as the canonical ensemble [20–22] and that the quantum states before and after the operation are both pure states. Thus, by applying the result (2) to a sequence of operations, we obtain the second law of thermodynamics (see Fig. 1).

The physics behind the entropy increase (2) is the time-energy uncertainty principle in quantum mechanics, which requires that any operation during a time Δt causes the energy uncertainty about $\hbar/\Delta t$, where \hbar is Planck's constant [7]. In large systems, there exists an exponentially large number of many-body eigenstates within the energy window $\hbar/\Delta t$ which cannot be distinguished and hence contribute to the entropy increase.

To illustrate the physical origin of the entropy increase, let us consider a qubit with two energy eigenstates $|0\rangle$ and $|1\rangle$. Each quantum state, which is described by a 2×2 density matrix ρ , is represented by a point on or inside a unit sphere called the Bloch sphere [23] (see Fig. 2a). Here the x -, y -, and z -coordinates are $\text{tr}[\rho\sigma_a]$ ($a = 1, 2, 3$), where σ_a 's are the Pauli matrices. The entropy of each state depends only on its z -component and monotonically increases from the poles to the equatorial plane (see Fig. 2b).

During the unitary evolution with the time-independent Hamiltonian, a pure state traces a circle

around the z -axis which we call the quantum orbit. The corresponding mixed state ρ_{dec} is defined by eliminating the coherence between $|0\rangle$ and $|1\rangle$ or, equivalently, by projecting the quantum orbit onto the z -axis (see Fig. 2c).

A quantum operation, together with the change of the energy eigenbasis, causes a unitary transformation on the quantum orbit, which is represented by a rotation on the Bloch sphere. The quantum orbit is transformed to a circle around a different axis with ρ_{dec} changing into ρ'_{dec} (see Fig. 2d).

From this consideration, it is obvious that the entropy of ρ_{dec} never decreases after the operation because ρ_{dec} approaches the equatorial plane. For the pure states on the orbit, the entropy is more likely to increase than decrease (see Fig. 2d). The inequality (2) thus holds with more than 50% probability. We note that this argument is valid only if the quantum orbit never crosses the equatorial plane. However, this condition, in practice, does not impose any restriction in the thermodynamic limit because the equatorial plane, which corresponds to the infinite temperature, cannot be reached.

The asymmetry in the entropy change originates from the fact that the quantum orbit is restricted to a circle around the z -axis, which breaks the invariance of the Hilbert space under any unitary transformation. No matter how complex the system might be, the energy is conserved and the Hamiltonian is well-defined and hence gives the preferred basis, which restricts the possible quantum orbits. It is remarkable that the entropy increase thus results from the conservation of the energy.

The absence of Maxwell's demon [24–27] is also essential for the entropy increase. It is because there exist some timings at which the operation decreases the entropy even though the probability is less than 50% for a qubit system and vanishingly small for a high-dimensional Hilbert space as shown below. Thus, un-

less one is able to know all the information on the pure state and do infinitely-fine tuning on the timing of the operation, the entropy increase is unavoidable.

For the general case, where the dimension of the Hilbert space is d , the entropy increase becomes much more probable than for a qubit system. The decohered state ρ_{dec} is defined by eliminating all the coherence between many-body eigenstates involved in the pure state. Then the entropy of ρ_{dec} increases during any thermodynamic process in which ρ_{dec} changes into ρ'_{dec} : $S \leq S'_{\text{dec}}$, where $S'_{\text{dec}} \equiv S(\rho'_{\text{dec}})$, because ρ_{dec} approaches the equatorial plane (see section I of Supplementary Information for details). For the pure states, ignoring a non-extensive correction (see Methods Summary), we obtain $S' = S'_{\text{dec}}$ and thus $S \leq S'$ except for the probability of the order of $d^{-1/2}$. In many-body systems, this is exponentially small with the number of particles.

Finally we demonstrate our result for a system of hard-core bosons on a lattice. We place five bosons on twenty sites, which are arranged in a 4×5 rectangle (see Fig. 3a), where the boundary is free. The kinetic energy is given by $\hat{H}_{\text{kin}} = -J \sum_{\langle i,j \rangle} (\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i)$, where \hat{b}_i^\dagger and \hat{b}_i represent the creation and annihilation operators of the boson on site i and the sum is taken over all the nearest neighbors, which means that each boson can hop to adjacent sites and the energy accompanied by the hopping is $-J (< 0)$. The hard-core condition is imposed by requiring that more than one particle cannot reside on any single site. We introduce a linear potential h along the y -axis, which gives a tilting potential energy, $\hat{H}_{\text{pot}} = h \sum_i y_i \hat{n}_i$, where \hat{n}_i is the number of particles on site i and $y_i = 0, 1, 2$ and 3 is the y -coordinate of the site i as illustrated in Fig. 3a. Applying this linear potential is equivalent to tilting the rectangle up at one edge in the gravitational field as illustrated in Fig. 3b.

Initially, the linear potential is switched off and the quantum state is prepared in the 1000th energy eigenstate and thus stationary. The entropy of this state is $S = 0$, which is the minimum. The first operation is the quantum quench at time $t = 0$, which suddenly switches on the linear potential to $h = J$ as illustrated in Fig. 3c. The entropy after the quench is $S' = 7.15$ and obviously $S \leq S'$ holds.

The second operation is the quench at $t = \tau$, which is a sudden switch-off of the linear potential from $h = J$ to 0 (see Fig. 3c). The entropy after the second quench S'' is shown in Fig. 3d. For the quench after equilibration, S'' coincides with S''_{dec} apart from a finite-size correction and thus $S' \leq S''$ holds, where S''_{dec} is the entropy after the second quench assuming that all the coherence between many-body eigenstates is lost after the first quench. It is remarkable that the finite-size correction is universal and given by $\gamma - 1$, where $\gamma = 0.5772 \dots$ is Euler's constant (see Methods Summary), since it is

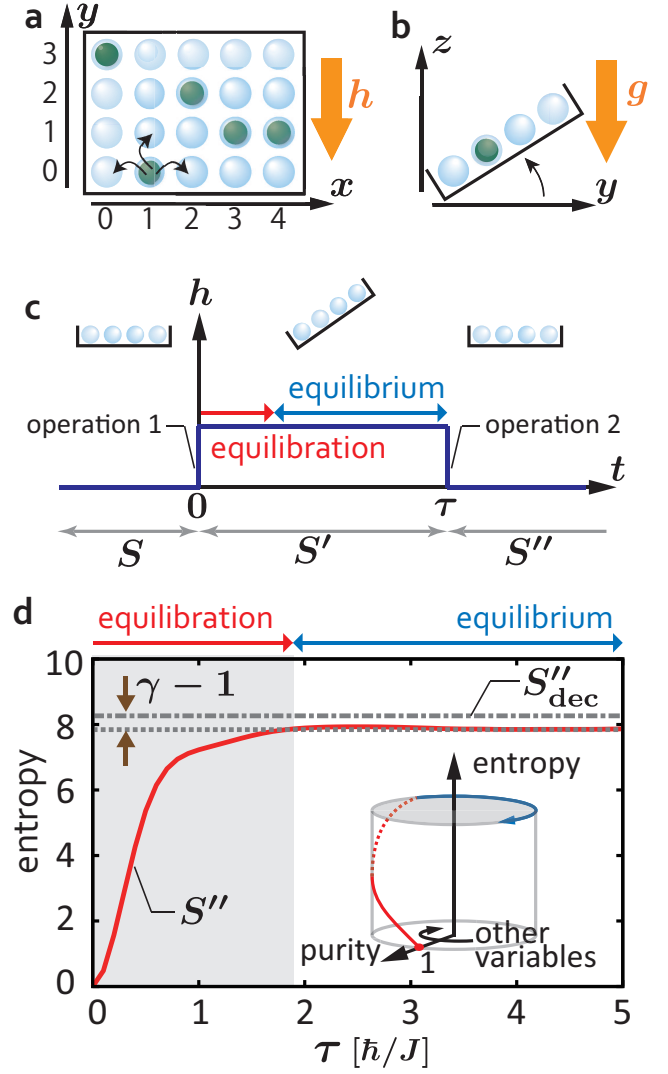


FIG. 3: **Numerical demonstration of the main result.** (a) The model. Five hard-core bosons are placed on the 4×5 sites whose boundary is free. The bosons can hop to adjacent sites. (b) Applying a linear potential h along the y axis tilts the potential energy of the rectangle up at one edge in the gravitational field g . (c) The protocol of the linear potential. For $t < 0$, we prepare the 1000th energy eigenstate, which is stationary. Two operations performed at $t = 0$ and τ are the switch-on and -off of h . (d) Entropy change after the second quench, or the switch-off of h at $t = \tau$, plotted against the quench time τ . The shaded area corresponds to the quench performed before equilibration (the corresponding region is indicated by the red arrow in (c)). The entropy in the unshaded area is independent of τ and equal to the one obtained for the decohered state except for the universal correction $\gamma - 1$. The inset shows a schematic figure of the entropy increase. A quantum state is confined in a constant-entropy surface after equilibration.

independent of the details of the system and processes.

The inset of Fig. 3d schematically illustrates a situation in which the quantum state is always pure and never converges to the decohered state during the unitary evolution. Nevertheless, the trajectory eventually approaches a constant-entropy surface whose entropy is the same as that of the decohered state. Our finding is that the quantum coherence between many-body eigenstates gives no more than a universal correction, which is negligible in the thermodynamic limit.

We remark the difference between equilibration and decoherence between the two quenches. So long as quantum-mechanical observables are concerned, we cannot distinguish them after the second quench [16, 17]. However, looking into the entropy, we can distinguish them (see Fig. 3d). The universal correction $\gamma - 1$ is the physical manifestation of the residual coherence and can be used as a criterion for judging the coherence of the system.

METHODS SUMMARY

Here we show Eq. (2) by considering the entropy after a given thermodynamic process (see process 1 in Fig. 1) as a function of the timing when the operation starts. By invoking the so-called replica trick [28], we have analytically derived the following relation by taking into account the leading-order finite-size correction:

$$\langle S' \rangle = S'_{\text{dec}} + \gamma - 1, \quad (3)$$

where the average on the left-hand side represents the time average on the timing (see Supplementary Information section II). Moreover, we have shown $\sigma / \langle S' \rangle = O(d^{-1/2})$ where σ is the standard deviation of S' and d is the dimension of the Hilbert space. Since d grows exponentially with the number of particles, this means that $S' = S'_{\text{dec}} + \gamma - 1$ holds with almost unit probability for any timing of the operation in many-body systems. Furthermore, since the finite-size effect $\gamma - 1$ is a universal constant, it can be ignored in the thermodynamic limit independently of the details of the system and processes, and thus we obtain $S' = S'_{\text{dec}} \geq S$ for almost every timing of the operation. It is reasonable on physical grounds to consider that the exceptional timings correspond to either before equilibration or on revivals after equilibration. Thus, we conclude that the entropy never decreases during any thermodynamic process between two pure states at equilibrium in the thermodynamic limit.

ACKNOWLEDGEMENT

Fruitful discussions with Takahiro Sagawa are gratefully acknowledged. This work was supported by

KAKENHI 22340114, a Grant-in-Aid for Scientific Research on Innovation Areas "Topological Quantum Phenomena" (KAKENHI 22103005), a Global COE Program "the Physical Sciences Frontier", and the Photon Frontier Network Program, from MEXT of Japan. T.N.I. acknowledges the JSPS for financial support (Grant No. 248408).

NOTE ADDED

After completion of this work, we became aware of an independent work by Hal Tasaki [29], where the second law of thermodynamics for pure states is addressed in terms of the energy.

-
- [1] Layzer, D. The arrow of time. *Sci. Am.* **233**, 56-69 (1975).
 - [2] Landau, L. D. & Lifshitz, L. M. *Statistical Physics*. (Butterworth-Heinemann, 1984), Vol. 5.
 - [3] Čápek, V. & Sheehan, D. P. *Challenges to the Second Law of Thermodynamics Theory and Experiment Fundamental Theories of Physics Volume 146*. (Springer 2005).
 - [4] Prigogine, I. *From Being to Becoming*. (Freeman, San Francisco, 1980).
 - [5] Breuer, H.-P. & Petruccione, F. *The Theory of Open Quantum Systems*. (Oxford University Press, 2002).
 - [6] Gemmer, J., Michel, M. & Mahler, G. *Quantum Thermodynamics, Lecture Notes in Physics Volume 784*. (Springer 2009).
 - [7] Landau, L. D. & Lifshitz, L. M. *Quantum Mechanics Non-Relativistic Theory* (Butterworth-Heinemann, 1981), Vol. 3.
 - [8] Greiner, M., Mandel, O., Hänsch, T. W. & Bloch, I. Collapse and revival of the matter wave field of a Bose-Einstein condensate. *Nature* **419**, 51-54 (2002).
 - [9] Kinoshita, T., Wenger T. & Weiss, D. S. A quantum Newton's cradle. *Nature* **440**, 900-903 (2006).
 - [10] Wieman, C. E., Pritchard, D. E. & Wineland, D. J. Atom cooling, trapping, and quantum manipulation. *Rev. Mod. Phys.* **71**, S253-S262 (1999).
 - [11] Serwane, F., Zürn, G., Lompe, T., Ottenstein, T. B., Wenz, A. N. & Jochim, S. Deterministic Preparation of a Tunable Few-Fermion System. *Science* **332**, 336-338 (2011).
 - [12] Korenblit, S., Kafri, D., Campbell, W. C., Islam, R., Edwards, E. E., Gong, Z.-X., Lin, G.-D., Duan, L.-M., Kim, J., Kim, K. & Monroe, C. Quantum Simulation of Spin Models on an Arbitrary Lattice with Trapped Ions. *New J. Phys.* **14**, 095024 (2012).
 - [13] Polkovnikov, A. Microscopic diagonal entropy and its connection to basic thermodynamic relations. *Ann. Phys. (N. Y.)* **326**, 486-499 (2011).
 - [14] Santos, L. F., Polkovnikov, A. & Rigol, M. Entropy of Isolated Quantum Systems after a Quench. *Phys. Rev. Lett.* **107**, 040601 (2011).
 - [15] Polkovnikov, A., Sengupta, K., Silva, A & Vengalattore, M. Colloquium: Nonequilibrium dynamics of closed interacting quantum systems. *Rev. Mod. Phys.* **83**, 863-883 (2011).

- [16] Rigol, M., Dunjko, V. & Olshanii, M. Thermalization and its mechanism for generic isolated quantum systems. *Nature* **452**, 854-858 (2008).
- [17] Reimann, P. Foundation of Statistical Mechanics under Experimentally Realistic Conditions. *Phys. Rev. Lett.* **101**, 190403 (2008).
- [18] Trotzky S., Chen Y-A., Flesch A., McCulloch I. P., Schollwöck, U., Eisert, J. & Bloch, I. Probing the relaxation towards equilibrium in an isolated strongly correlated 1D Bose gas. *Nature Physics* **8**, 325-330 (2012).
- [19] von Neumann, J. Proof of the ergodic theorem and the H-theorem in quantum mechanics (Translation of: Beweis des Ergodensatzes und des H-Theorems in der neuen Mechanik.) *Eur. Phys. J. H* **35**, 201-237 (2010). [The German original was published in *Zeitschrift für Physik* **57**, 30-70 (1929).]
- [20] Jarzynski, C. Nonequilibrium Equality for Free Energy Differences. *Phys. Rev. Lett.* **78**, 2690-2693 (1997).
- [21] Crooks, G. E. Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences. *Phys. Rev. E* **60**, 2721-2726 (1999).
- [22] Dorner, R., Goold, J., Cormick, C., Paternostro M. & Vedral V. Emergent Thermodynamics in a Quenched Quantum Many-Body System. *Phys. Rev. Lett.* **109**, 160601 (2012).
- [23] Nielsen M. A., & Chuang, I. L. *Quantum Computation and Quantum Information*. (Cambridge University Press, 2000).
- [24] Leff, H. & Rex, A. F. *Maxwell's Demon 2: Entropy, Classical and Quantum Information, Computing*. (Taylor and Francis, 2002), 2nd Edition.
- [25] Maruyama, K., Nori, F. & Vedral, V. The physics of Maxwell's demon and information. *Rev. Mod. Phys.* **81**, 1-23 (2009).
- [26] Sagawa, T. & Ueda, M. Minimal energy cost for thermodynamic information processing: measurement and information erasure. *Phys. Rev. Lett.* **102**, 250602 (2009).
- [27] Toyabe, S., Sagawa, T., Ueda, M., Muneyuki, E. & Sano, M. Experimental demonstration of information-to-energy conversion and validation of the generalized Jarzynski equality. *Nature Physics* **6**, 988-992 (2010).
- [28] Edwards, S. F. & Anderson, P. W. Theory of spin glasses *J. Phys. F: Met. Phys.* **5** 965 (1975).
- [29] Tasaki, H. The second law of Thermodynamics as a theorem in quantum mechanics. *arXiv:cond-mat/0011321* (2000).

SUPPLEMENTARY INFORMATION (Emergent Second Law in Pure Quantum States)

This supplementary material includes four sections. First, we demonstrate how the geometrical concepts utilized in a qubit system are generalized to higher dimensions. Second, we show the results presented in Methods Summary in the manuscript. Third, we provide supplementary numerical data that verify the universality of the non-extensive correction to the entropy after a thermodynamic process. Last, we apply our method to a closely related quantity, the diagonal Rényi entropy for which we can also find universal corrections. This result suggests that our non-extensive universal correction appears for a rather broad class of diagonal entropies.

A. GEOMETRICAL INTERPRETATION FOR THE HIGHER-DIMENSIONAL HILBERT SPACE

In this section, we describe the quantum orbit and the operation in the high-dimensional “Bloch sphere”. Then we illustrate that the entropy never decreases for the decohered state. With the results shown in Section B, this leads to the entropy increase for pure states.

A-1. Bloch sphere

Let d be the dimension of the Hilbert space. Every quantum state is described by a $d \times d$ density matrix ρ . The density matrix ρ is Hermitian with unit trace. As a convenient orthonormal basis of the traceless $d \times d$ Hermitian matrices, we adopt the generalized Gell-Mann matrices λ_a ($a = 1, 2, \dots, d^2 - 1$) [1]. The first $d - 1$ matrices are diagonal and analogous to σ_3 , and the others are off-diagonal and analogous to σ_1 and σ_2 , where σ_a 's ($a = 1, 2, 3$) are the Pauli matrices. Thus, each density matrix ρ is parametrized by $d^2 - 1$ variables $x_a = \text{tr}[\rho \lambda_a]$ ($a = 1, \dots, d^2 - 1$) and represented by a point in the $(d^2 - 1)$ -dimensional Euclidean space. We note that all these points, which constitute the “Bloch sphere” in the $(d^2 - 1)$ -dimensional Euclidean space, do not form a $(d^2 - 2)$ -sphere for $d > 2$ unlike the qubit system for $d = 2$ [2].

A-2. Quantum orbit

During the time evolution with a fixed Hamiltonian, a quantum state traces a quantum orbit in the “Bloch sphere”. In the energy eigenbasis representation, the first $d - 1$ components, x_a 's ($a = 1, 2, \dots, d - 1$), do not change whereas the others, x_a 's ($a = d, d +$

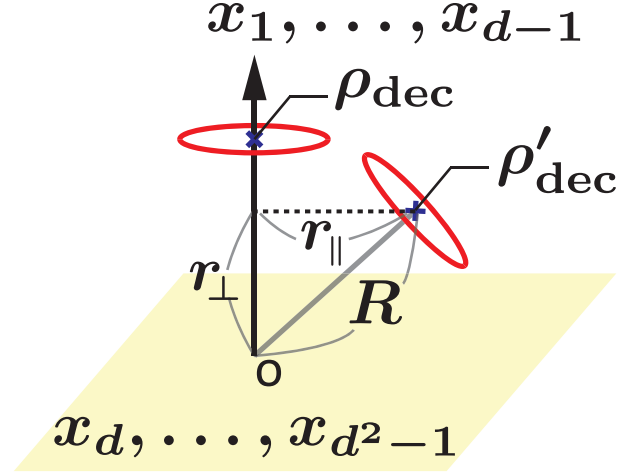


FIG. A.1: **Geometry in higher dimensions.** In higher dimensions, the quantum orbit is described in the subspace perpendicular to the $(d - 1)$ -dimensional plane spanned by the x_a -axes ($a = 1, 2, \dots, d - 1$). The operation preserves the distance from the origin $R = \sqrt{\sum_{a=1}^{d^2-1} x_a^2}$, but decreases the distance from the equatorial plane $r_{\perp} = \sqrt{\sum_{a=1}^{d-1} x_a^2}$. The approach to the equatorial plane implies an increase in entropy.

$1, \dots, d^2 - 1$), do. Thus, the quantum orbit is restricted to a subspace, which is perpendicular to the $(d - 1)$ -dimensional plane spanned by the x_a -axes ($a = 1, \dots, d - 1$) (see Fig. A.1).

The decohered state ρ_{dec} is the projection of the orbit onto the subspace, in which no coherence exists between energy eigenstates. We note that each point on the quantum orbit is equidistant from ρ_{dec} because the first $d - 1$ components, x_a 's ($a = 1, 2, \dots, d - 1$), and the distance from the origin $R = \sqrt{\sum_{a=1}^{d^2-1} x_a^2}$ are preserved under unitary evolutions.

A-3. Operation

The operation, which can be implemented by a change in control parameters, is represented by a $d \times d$ unitary matrix. The change of the energy eigenbasis during the operation can also be described by a unitary matrix. The combination of these two unitary matrices produces a single unitary matrix acting on the quantum orbit. Due to the unitarity, the distance from the origin R and the distance between ρ_{dec} and each state on the orbit are preserved.

A-4. Monotonicity of the entropy of the decohered state

The equatorial plane of the Bloch sphere is generalized to be the plane where $x_a = 0$ for $a = 1, 2, \dots, d-1$. The distance from the plane is defined by $r_\perp \equiv \sqrt{\sum_{a=1}^{d-1} x_a^2}$. We also define $r_\parallel \equiv \sqrt{\sum_{a=d}^{d^2-1} x_a^2}$ as the distance from the subspace spanned by x_a 's ($a = 1, 2, \dots, d-1$). Then the relation $R^2 = r_\perp^2 + r_\parallel^2$ holds.

The decohered state satisfies $r_\parallel = 0$ by definition and thus $R = r_\perp$. Since R is preserved during the operation, $r_\perp \geq r'_\perp$ follows. This means that the decohered state approaches the equatorial plane during the operation, resulting in an increase in entropy.

B. ENTROPY AFTER A THERMODYNAMIC PROCESS

In this section, we analyze the entropy after an arbitrary thermodynamic process as a function of the timing when the operation starts. The infinite-time average involves S'_{dec} and the universal correction $\gamma - 1$. The infinite-time variance is shown to decrease exponentially with the system size.

B-1. Setup

The Hamiltonian is given as follows (see Fig. B.1):

$$H(t) = \begin{cases} H & t \leq \tau; \\ H_{\text{op}}(t) & \tau \leq t \leq \tau + \Delta\tau; \\ H' & \tau + \Delta\tau \leq t, \end{cases} \quad (\text{B.1})$$

where we assume $H_{\text{op}}(\tau) = H$ and $H_{\text{op}}(\tau + \Delta\tau) = H'$. Let $\{|E_n\rangle\}$ and $\{|E'_n\rangle\}$ be the set of eigenstates of H and that of H' , respectively. To ensure equilibration, H and H' are assumed to be nonintegrable. The initial state is assumed to be pure and thus expanded in terms of the energy eigenstates of H : $|\psi\rangle = \sum_n c_n |E_n\rangle$. We also assume that the number of the superposed eigenstates is large and the inverse participation ratio (IPR) $Q \equiv \sum_n |c_n|^4$ is of the order of d^{-1} where d is the dimension of the Hilbert space and grows exponentially with the system size. The IPR plays a role as the expansion parameter in the following discussion.

At time $t = \tau$, each eigenstate has acquired a phase proportional to its eigenenergy: $|\psi(\tau)\rangle = \sum_n c_n e^{-iE_n\tau} |E_n\rangle$, where Planck's constant is set to unity. The time evolution from τ to $\tau + \Delta\tau$ is described by a unitary operation $V \equiv \mathcal{T} \exp\left(-i \int_0^{\Delta\tau} H_{\text{op}}(\tau + t) dt\right)$, where \mathcal{T} is the time-ordering operator. Thus the quantum state at $t = \tau + \Delta\tau$ is given by $|\psi(\tau + \Delta\tau)\rangle = \sum_n c_n e^{-iE_n\tau} V |E_n\rangle$. Expressing this state in terms of the eigenbasis of H' , we obtain $|\psi(\tau + \Delta\tau)\rangle = \sum_n c'_n |E'_n\rangle$

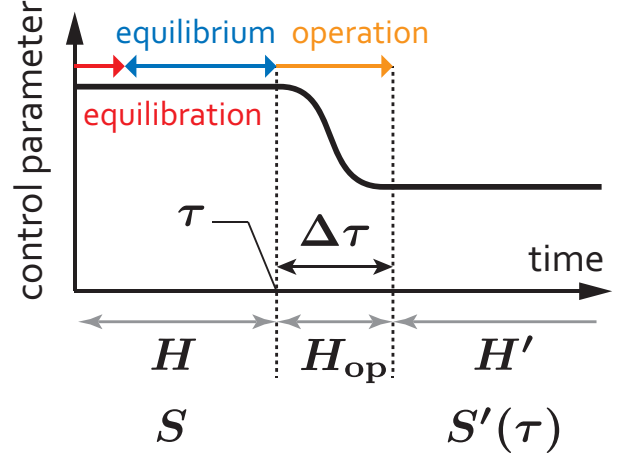


FIG. B.1: **Control protocol.** First, an initial pure state with Hamiltonian H undergoes equilibration and reaches equilibrium. Then the operation starts at $t = \tau$ which smoothly transforms H to the final Hamiltonian H' . The entropy S' after the operation, in general, depends on τ . However, for τ greater than the equilibration time, S' is expected to be independent of τ apart from small fluctuations due to a finite-size effect.

where $c'_n = \sum_m c_m e^{-iE_m\tau} U_{nm}$ and $U_{mn} \equiv \langle E'_m | V | E_n \rangle$. Note that U_{mn} 's denote the transition amplitudes between pairs of the eigenstates before and after the operation.

B-2. Entropy after the operation

The entropy after the operation depends on the timing when the operation is performed, and is given by

$$S'(\tau) = - \sum_n |c'_n|^2 \ln |c'_n|^2. \quad (\text{B.2})$$

Since we are interested in the operation performed on the pure state at equilibrium, we calculate $S'(\tau)$ for sufficiently large τ . To examine this limit, we have only to calculate the long-time average on τ , or $\langle S'(\tau) \rangle_\tau$. Here $\langle \dots \rangle_\tau$ means $\lim_{T \rightarrow \infty} T^{-1} \int_0^T \dots d\tau$. We will also show below that the fluctuation of $S'(\tau)$ actually vanishes for large systems. To calculate the long-time average of each term on the right-hand side of Eq. (B.2), we first consider the probability distribution of $|c'_n|^2$.

B-3. Moments of the population of each eigenstate after the operation

Here we show that the population of each eigenstate, $|c'_n|^2$, after the operation obeys the exponential distribution. For this purpose, we analyze the moments of the

k -th order:

$$\begin{aligned} & \langle |c'_n|^{2k} \rangle_\tau \\ &= \sum_{\substack{m_1, \dots, m_k \\ l_1, \dots, l_k}} \left[\prod_{j=1}^k U_{nm_j} U_{nl_j}^* c_{m_j} c_{l_j}^* \right] \langle e^{-i(\sum_{j=1}^k \phi_{m_j} - \sum_{j=1}^k \phi_{l_j})} \rangle, \end{aligned} \quad (\text{B.3})$$

where $\phi_m \equiv E_m \tau \pmod{2\pi}$ and $\langle \dots \rangle$ denotes the average over ϕ_m 's under the assumptions that each ϕ_m is uniformly distributed over $[0, 2\pi)$ and that ϕ_m and ϕ_l are independent for $m \neq l$. The replacement of $\langle \dots \rangle_\tau$ with $\langle \dots \rangle$ is justified for nonintegrable systems, where the energy spectrum is sufficiently complex [3].

We note the following relation:

$$\langle e^{-i(\sum_{j=1}^k \phi_{m_j} - \sum_{j=1}^k \phi_{l_j})} \rangle = \sum_{\sigma \in \mathcal{S}_k} \prod_{j=1}^k \delta_{m_j l_{\sigma(j)}} + (\text{corrections}), \quad (\text{B.4})$$

where \mathcal{S}_k is the symmetric group on k elements. It can be shown that the correction terms give contributions smaller than the first term on the right-hand side of Eq. (B.4) roughly by a factor of $Q_n \equiv \sum_m (|U_{nm}|^2 |c_m|^2)^2$. Here Q_n is a kind of the IPR defined above and Q_n^{-1} represents an effective number of the eigenstates that can evolve into $|E'_n\rangle$ by the unitary operation V .

Let us illustrate this for $k = 2$. Writing out the terms explicitly, we have $\langle e^{-i(\phi_{m_1} + \phi_{m_2} - \phi_{l_1} - \phi_{l_2})} \rangle = \delta_{m_1 l_1} \delta_{m_2 l_2} + \delta_{m_1 l_2} \delta_{m_2 l_1} - \delta_{m_1 m_2} \delta_{m_1 l_1} \delta_{m_2 l_2}$. The third term, which is the only correction term in this case, corrects the double counting in the first and second term for $m_1 = m_2$. In such a manner, the correction terms in Eq. (B.4) have more Kronecker's deltas which make the correction terms smaller by a factor of Q_n .

We assume that the operation is such that $Q_n \ll 1$. This condition is satisfied unless $\Delta\tau = \infty$ or $H_{\text{op}}(t) = H = H'$, because, in large systems, the energy spectrum so dense that there should be a number of transitions between many-body eigenstates. We note that $\Delta\tau = \infty$ corresponds to the adiabatic process, which causes no transition between many-body eigenstates. Although our discussion cannot be applied to this case, we obtain $S = S'$ by definition, which is consistent with the fact that the entropy is invariant for quasi-static processes in isolated systems. As for $H_{\text{op}}(t) = H = H'$, the entropy is invariant for lack of any operation.

Substituting Eq. (B.4) into Eq. (B.5) and ignoring the correction terms, we obtain

$$\langle |c'_n|^{2k} \rangle_\tau = k! \mu_n^k, \quad (\text{B.5})$$

where $\mu_n \equiv \sum_m |U_{nm}|^2 |c_m|^2$.

To see the physical meaning of μ_n , let us imagine that the initial state has no coherence between energy eigenstates. The decohered state is represented by a density matrix $\rho_{\text{dec}} = \sum_n |c_n|^2 |E_n\rangle \langle E_n|$. Due to the absence of

coherence, this state is stationary. After the operation, it becomes $\rho'_{\text{dec}} = V \rho_{\text{dec}} V^\dagger$, and the population of each eigenstate $|E'_n\rangle$ is $\langle E'_n | \rho'_{\text{dec}} | E'_n \rangle = \mu_n$. Thus, μ_n corresponds to the population of $|E'_n\rangle$ for the decohered initial state. We note that the factor $k!$ in Eq. (B.5) would be absent if it were not for coherence between energy eigenstates.

Equation (B.5) means that $|c'_n|^2$ obeys an exponential distribution

$$P(|c'_n|^2) = e^{-|c'_n|^2/\mu_n}/\mu_n, \quad (\text{B.6})$$

whose mean and variance are μ_n and μ_n^2 , respectively.

B-4. Average of the entropy after the operation

We obtain the long-time average of $S'(\tau)$ by taking the average over the exponential distribution [Eq. (B.6)]:

$$\begin{aligned} \langle S'(\tau) \rangle_\tau &= - \sum_n \int_0^\infty |c'_n|^2 \ln |c'_n|^2 \frac{e^{-|c'_n|^2/\mu_n}}{\mu_n} d|c'_n|^2 \\ &= - \sum_n \mu_n \ln \mu_n + \gamma - 1 \\ &= S'_{\text{dec}} + \gamma - 1, \end{aligned} \quad (\text{B.7})$$

where S'_{dec} is the entropy of ρ'_{dec} and γ is Euler's constant. Interestingly, the constant $\gamma - 1$ does not depend on details of the system and the operation, whereas S'_{dec} does. We note that S'_{dec} is extensive [4], and $S \leq S'_{\text{dec}}$ since $|U_{mn}|^2$ is doubly-stochastic [5]. Thus, the second law is obtained for large systems, where the constant $\gamma - 1$ can be ignored.

To make it clear that the universal constant $\gamma - 1$ originates from the factorial $k!$ in Eq. (B.5), or, equivalently, from the quantum coherence between energy eigenstates, we provide another derivation by invoking the so-called replica trick [6], which relies on the analytic continuation of Eq. (B.5) to $k = 0$:

$$\begin{aligned} \langle S(\tau) \rangle_\tau &= - \sum_n \lim_{k \rightarrow 0} \frac{\langle |c'_n|^{2(k+1)} \rangle_\tau - \langle |c'_n|^2 \rangle_\tau}{k} \\ &= - \sum_n \lim_{k \rightarrow 0} \frac{\Gamma(k+2) \mu_n^{k+1} - \mu_n}{k} \\ &= - \sum_n \mu_n \ln \mu_n + \gamma - 1. \end{aligned} \quad (\text{B.8})$$

It is clear from this derivation that the universal constant arises from $k! = \Gamma(k+1)$.

B-5. Variance of the entropy after the operation

Finally, we justify our conjecture that $S'(\tau)$ is effectively independent of τ if τ is larger than the equilibration time and the operation is performed on the pure

state at equilibrium. For this purpose, we show that the variance of $S'(\tau)$ decreases exponentially with the

system size.

We begin by calculating the moments for $n \neq \tilde{n}$,

$$\langle |c'_n|^{2k} |c'_{\tilde{n}}|^{2\tilde{k}} \rangle_\tau = \sum_{\substack{m_1, \dots, m_k \\ l_1, \dots, l_k}} \sum_{\substack{\tilde{m}_1, \dots, \tilde{m}_{\tilde{k}} \\ \tilde{l}_1, \dots, \tilde{l}_{\tilde{k}}}} \left[\prod_{j=1}^k U_{nm_j} U_{nl_j}^* c_{m_j} c_{l_j}^* \right] \left[\prod_{\tilde{j}=1}^{\tilde{k}} U_{\tilde{n}\tilde{m}_{\tilde{j}}} U_{\tilde{n}\tilde{l}_{\tilde{j}}}^* c_{\tilde{m}_{\tilde{j}}} c_{\tilde{l}_{\tilde{j}}}^* \right] \left\langle e^{-i \left(\sum_{j=1}^k \phi_{m_j} + \sum_{\tilde{j}=1}^{\tilde{k}} \phi_{\tilde{m}_{\tilde{j}}} - \sum_{j=1}^k \phi_{l_j} - \sum_{\tilde{j}=1}^{\tilde{k}} \phi_{\tilde{l}_{\tilde{j}}} \right)} \right\rangle. \quad (\text{B.9})$$

We assume $k \leq \tilde{k}$ without loss of generality. Substituting Eq. (B.4) into Eq. (B.9) and ignoring the correction terms, we obtain

$$\langle |c'_n|^{2k} |c'_{\tilde{n}}|^{2\tilde{k}} \rangle_\tau = k! \tilde{k}! \sum_{q=0}^k \binom{k}{q} \binom{\tilde{k}}{q} \mu_n^{k-q} \mu_{\tilde{n}}^{\tilde{k}-q} |\nu_{n\tilde{n}}|^{2q}, \quad (\text{B.10})$$

where $\nu_{n\tilde{n}} \equiv \sum_m U_{nm} U_{\tilde{n}m}^* |c_m|^2$ are the off-diagonal elements of ρ'_{dec} . Equation (B.10) can be expressed as

$$\begin{aligned} \langle |c'_n|^{2k} |c'_{\tilde{n}}|^{2\tilde{k}} \rangle_\tau &= \left[\Gamma(k+1) \mu_n^k \right] \left[\Gamma(\tilde{k}+1) \mu_{\tilde{n}}^{\tilde{k}} \right] {}_2F_1(-k, -\tilde{k}, 1; R_{n\tilde{n}}), \end{aligned} \quad (\text{B.11})$$

where ${}_2F_1(a, b, c; z)$ is the Gauss hypergeometric function and $R_{n\tilde{n}} \equiv |\nu_{n\tilde{n}}|^2 / (\mu_n \mu_{\tilde{n}})$. We note that $R_{n\tilde{n}} \sim Q \ll 1$ because $\sum_{n, \tilde{n}} |\nu_{n\tilde{n}}|^2 = \sum_n |c_n|^4 = Q \ll 1$, while $\sum_{n, \tilde{n}} \mu_n \mu_{\tilde{n}} = 1$. Thus, the first-order approximation is justified, which leads to

$$\langle |c'_n|^{2k} |c'_{\tilde{n}}|^{2\tilde{k}} \rangle_\tau = \left[\Gamma(k+1) \mu_n^k \right] \left[\Gamma(\tilde{k}+1) \mu_{\tilde{n}}^{\tilde{k}} \right] (1 + k\tilde{k} R_{n\tilde{n}}). \quad (\text{B.12})$$

By invoking the replica trick, we have for $n \neq \tilde{n}$

$$\langle |c'_n|^2 \ln |c'_n|^2 |c'_{\tilde{n}}|^2 \ln |c'_{\tilde{n}}|^2 \rangle_\tau - \langle |c'_n|^2 \ln |c'_n|^2 \rangle_\tau \langle |c'_{\tilde{n}}|^2 \ln |c'_{\tilde{n}}|^2 \rangle_\tau = R_{n\tilde{n}} \cdot O\left((d^{-1} \ln d)^2\right), \quad (\text{B.13})$$

where we assume $\mu_n = O(d^{-1})$ since $\sum_n \mu_n = 1$. Finally, we obtain the variance of $S'(\tau)$:

$$\begin{aligned} \sigma^2 &\equiv \langle S'(\tau)^2 \rangle_\tau - \langle S'(\tau) \rangle_\tau^2 \\ &= \sum_n \left[\langle (|c'_n|^2 \ln |c'_n|^2)^2 \rangle_\tau - \langle |c'_n|^2 \ln |c'_n|^2 \rangle_\tau^2 \right] \\ &\quad + \sum_{n, \tilde{n}} \left[\langle |c'_n|^2 \ln |c'_n|^2 |c'_{\tilde{n}}|^2 \ln |c'_{\tilde{n}}|^2 \rangle_\tau \right. \\ &\quad \left. - \langle |c'_n|^2 \ln |c'_n|^2 \rangle_\tau \langle |c'_{\tilde{n}}|^2 \ln |c'_{\tilde{n}}|^2 \rangle_\tau \right] \\ &= O\left(d \cdot (d \ln d)^2\right) + O\left(d^2 \cdot d^{-1} (d \ln d)^2\right) \\ &= O\left(d^{-1} (\ln d)^2\right), \end{aligned} \quad (\text{B.14})$$

where we have used $\sum_n = O(d)$ and $R_{n\tilde{n}} = O(d^{-1})$. Since $\langle S'(\tau) \rangle_\tau = O(\ln d)$, the variance vanishes exponentially with the number of particles N in the system:

$$\frac{\sigma}{\langle S'(\tau) \rangle_\tau} = O(d^{-1/2}) = O(e^{-N}). \quad (\text{B.15})$$

According to the Chebyshev's inequality, the probability with which $S'(\tau)$ deviates significantly from $\langle S'(\tau) \rangle$ becomes exponentially small as the system size increases [3, 7].

C. UNIVERSALITY OF THE NON-EXTENSIVE CORRECTION

We provide further evidence for the universality of the correction $\gamma - 1$. The model and the protocol are the same as in the manuscript. We focus on the second operation and plot $S'' - S''_{\text{dec}}$ with the error bar σ for various values of h (see Fig. C.1). Here S'' and σ are calculated by the average and the standard deviation of $S''(\tau)$ in the time interval $[50, 100]$ in units of \hbar/J . We can see that the universal correction coincides with $\gamma - 1$ independently of the value of h .

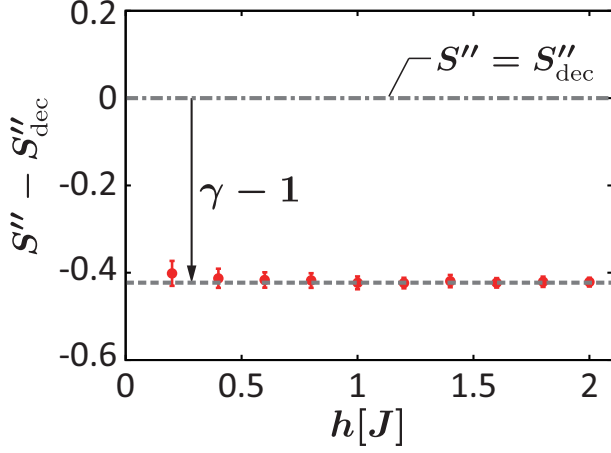


FIG. C.1: **Universality of $\gamma - 1$.** S'' averaged over $\tau \in [50, 100]\hbar/J$ minus S''_{dec} plotted for various h . The error bar is the standard deviation. Note that $\gamma - 1$ is independent of h .

D. THE DIAGONAL RÉNYI ENTROPY

Here we show that the universal correction can also be seen in the diagonal Rényi entropy, which is defined as

$$S_k \equiv \frac{\ln \left(\sum_n |c_n|^{2k} \right)}{1 - k} \quad (\text{D.1})$$

where k is an integer larger than 1. The analytic continuation $k \rightarrow 1$ gives the entropy discussed above. We also note that $S_2 = -\ln Q$. By invoking the replica trick and the approximation used in calculating the variance of the entropy, we obtain

$$\langle S'_k(\tau) \rangle_\tau = S'_{k,\text{dec}} + \frac{\ln k!}{1 - k}, \quad (\text{D.2})$$

where $S'_{k,\text{dec}} \equiv \ln \left(\sum_n \mu_n^k \right) / (1 - k)$ is the diagonal-Rényi-entropy counterpart of S'_{dec} . The second term on the right-hand side of Eq. (D.2) is independent of the details of the system and processes and thus universal. Taking the limit of $k \rightarrow 1$ in Eq. (D.2), we reproduce the result (B.7).

Equation (D.2) can also be obtained in a different way. We introduce the generalized IPR as $Q^{(k)} \equiv \sum_n |c_n|^{2k}$. Then, from Eq. (B.5), we have

$$\langle Q^{(k)'}(\tau) \rangle_\tau = k! Q^{(k)'}_{\text{dec}}, \quad (\text{D.3})$$

where $Q^{(k)'}_{\text{dec}} \equiv \sum_n \mu_n^k$. Taking the logarithm of both sides and interchange the logarithm and the average on the left-hand side, we obtain Eq. (D.2).

-
- [1] Georgi, H. *Lie Algebras In Particle Physics: from Isospin To Unified Theories*. (Westview Press, 1999).
 - [2] Kimura, G. The Bloch vector for N -level systems. *Phys. Lett. A* **314** 339-349 (2003).
 - [3] Reimann, P. Foundation of Statistical Mechanics under Experimentally Realistic Conditions *Phys. Rev. Lett.* **101** 190403 (2008).
 - [4] Polkovnikov, A. Microscopic diagonal entropy and its connection to basic thermodynamic relations. *Annals of*

- Physics* **326** 486-499 (2011).
- [5] Bhatia, R. *Matrix Analysis* (Springer, 1996).
- [6] Edwards, S. F. & Anderson, P. W. Theory of spin glasses *J. Phys. F: Met. Phys.* **5** 965 (1975).
- [7] Tasaki, H. From Quantum Dynamics to the Canonical Distribution: General Picture and a Rigorous Example *Phys. Rev. Lett.* **80** 1373-1376 (1998).